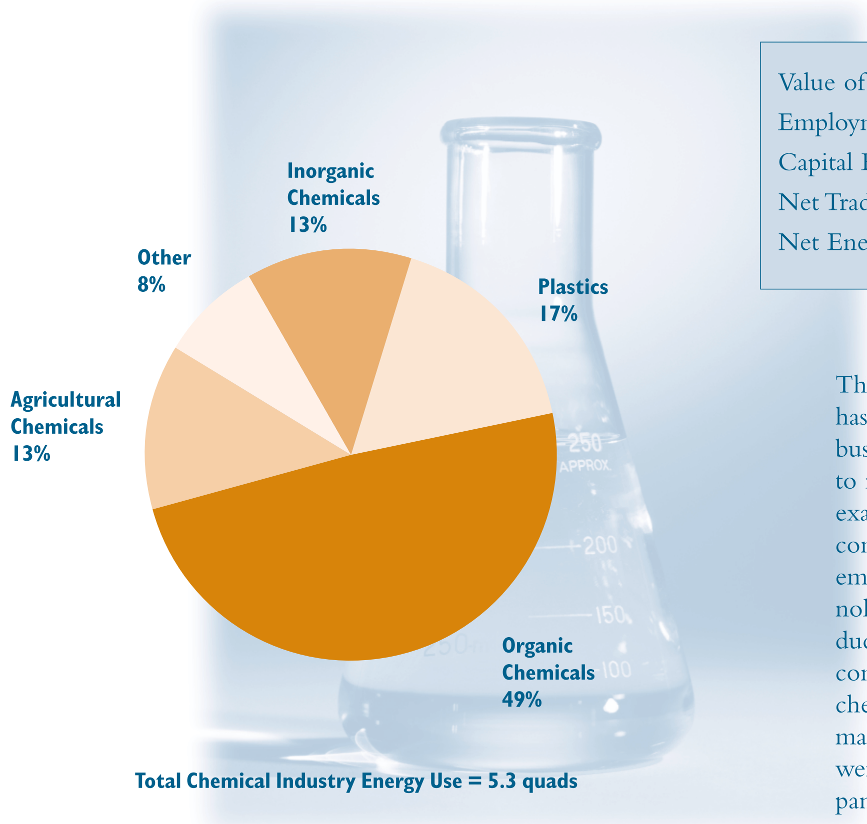
The United States chemical industry is the world's largest, accounting for 25% of world chemical production. Chemicals are the building blocks of many products that meet our most fundamental needs for food, shelter, and health, as well as products vital to such advanced technologies as computing, telecommunications, and biotechnology.

PROFILE

Chemical Industry



Total Chemical Industry Energy Use = 5.3 quads

Value of Shipments	$418.4 billion
Employment	877,100
Capital Expenditures	$21.3 billion
Net Trade Balance	$18.9 billion
Net Energy Consumption	5.3 quads

The United States chemical industry has been changing the way it does business as part of its continued efforts to remain globally competitive. For example, many of the industry's large companies have been increasing emphasis on life sciences and biotechnology. In addition, the chemical production process is becoming more comprehensive. Traditionally, some chemical companies manufactured primary or commodity chemicals, which were then sold to other chemical companies to refine into intermediate and specialty chemicals. Today, more companies are manufacturing the entire spectrum of chemical products and marketing them directly to consumers, bypassing the secondary chemical companies and adding value to their own products.

MANUFACTURING AND OPERATIONS

About 9,000 chemical facilities account for more than 70,000 products that are essential to many industries such as pharmaceuticals, automobiles, textiles, furniture, paint, paper, electronics, agriculture, construction, appliances, and services. Investments in new plants and equipment reached $21 billion in 1997, up from $16.4 billion in 1992. Research and development funding reached an estimated $18.6 billion in 1997, with pharmaceuticals R&D accounting for $11.6 billion of that amount. The chemical industry continues to enjoy steady growth, contributing 2.1% of the annual U.S. GDP. Production in the overall chemical industry rose 5.1% in 1997 from the previous year, and an estimated $418 billion worth of chemical products were shipped.

EMPLOYMENT

The chemical industry employs nearly a million people, almost half of whom work in chemical production. Approximately 90,000 chemists, engineers, and technicians are employed in R&D. More than 63% of chemical production is concentrated in ten states: Texas, New Jersey, Louisiana, Illinois, Ohio, California, North Carolina, Pennsylvania, New York, and South Carolina. Roughly 70% of basic chemicals are produced in the Gulf Coast region.

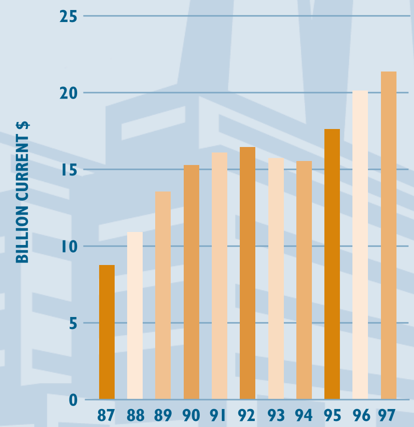
ENERGY

The chemical industry is energy-intensive, using energy as both fuel and feedstock. In 1994, the chemical industry consumed more than 5.3 quads of energy (the equivalent of over 2 million barrels of crude oil per day), which is approximately 25% of total manufacturing energy use. Of that 5.3 quads, over half was used for heat and power; the remaining energy was used as feedstock. The industry has made significant gains in energy efficiency, decreasing the energy consumed for fuel and power per unit of output by about 41% between 1974 and 1997.

ENVIRONMENT

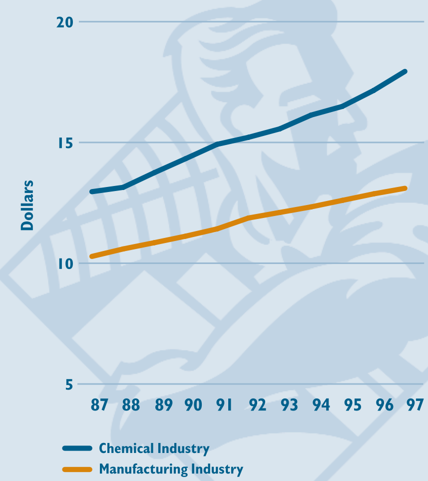
There are 16 major federal statutes as well as numerous state laws that impose significant compliance and reporting requirements on the industry. In addition, the industry's own voluntary program, Responsible Care®, further commits chemical companies to continuously improving their health, safety, and environmental performance in response to public concerns. The industry spent nearly $7 billion in 1994 to meet government requirements for pollution abatement and control. These expenditures are clearly making a difference. The industry decreased toxic releases 51% between 1988 and 1997, yet production rose 38% during that same time period.

CHEMICAL INDUSTRY INVESTMENT IN PLANTS & EQUIPMENT, 1987-1997



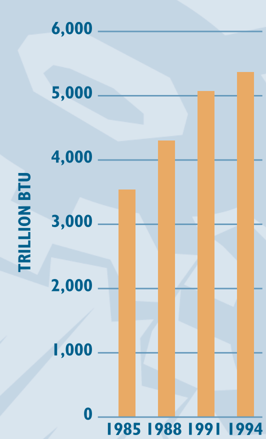
Source: U.S. Census Bureau

HOURLY EARNINGS: CHEMICAL INDUSTRY VS. MANUFACTURING, 1987-1997



Source: U.S. Census Bureau

CHEMICAL INDUSTRY ENERGY USE



Source: EIA, MECS

Industry Vision and Roadmaps

CHEMICAL INDUSTRY VISION

Partnerships between the chemical industry and OIT continue to pursue the goals set forth in the 1996 industry document, *Technology Vision 2020: The U.S. Chemical Industry.* Working with representatives from a wide variety of companies and associations, the chemical industry and OIT are developing a portfolio of manufacturing technologies that will ensure the continued global success of U.S. chemical companies and products. *Technology Vision 2020* identifies the following areas as critical to improving the industry's competitiveness:

- New chemical science and engineering technology
- Supply chain management
- Information systems
- Manufacturing and operations

CHEMICAL INDUSTRY ROADMAPS

Technology roadmaps in several critical areas describe the priorities and performance targets necessary to meet the challenges facing the industry and to achieve the goals outlined in *Technology Vision 2020.* These roadmaps will guide R&D efforts in the five critical areas outlined in the vision.

In the area of **chemical synthesis,** the roadmap for new process chemistry promotes the use of alternative processes and reaction media that are more environmentally benign than traditional methods and make more efficient use of raw materials. Catalysis is also an important factor in chemical synthesis. About 90% of chemical manufacturing processes and more than 20% of all industrial products in the United States

THE CHEMICAL INDUSTRY ROADMAPS ESTABLISH INDUSTRY-WIDE PRIORITIES AND PERFORMANCE TARGETS...

SAMPLE PERFORMANCE TARGETS

Computational Fluid Dynamics	• Shorten lead times (from research to final plant design) to 3-5 years • Shorten plant down times to 1% • Reduce separation energy use and improve separation efficiency by 20% • Increase reliability of design/reduce or eliminate design errors
Computational Chemistry	• Increase speed of performance by 2^{10} • Quantum scale—achieve 0.2kcal/mole accuracy for 20-30 heavy-atom systems and 1-2 kcal/mole accuracy for larger systems • Atomistic scale—routinely address systems of 1 million atoms/1,000 angstroms • Meso scale—predict continuum properties on scales as large as 10,000 nanometers with accuracy similar to atomistic level calculations
Materials Technology	• Reduce the use of nonreusable (nonsustainable) materials by 20% • Reduce CO_2 emissions per kWh by 30% by 2020 • Increase speed of testing of materials by an order of magnitude by 2020
Materials of Construction	• Minimize capital cost and energy consumption by 30% by 2020 • Maximize asset productivity by increasing uptime 25% and improving first-pass, first-quality yield by 20% • Protect the environment by containing the process with zero fugitive emissions, eliminating toxic discharges to the ground, and reducing hazardous wastes by 50% • Provide a safe operating environment with zero on-the-job injuries
Separations, Biocatalysis, and Reaction Engineering	• Achieve 30% reduction in relative indicators for material usage, energy use, water consumption, toxic dispersion, and pollutant dispersion
New Process Chemistry	• Reduce industry-wide energy intensity (energy per unit product) by 30% • Reduce total emissions and effluents from chemical manufacturing by 30% • Reduce cost of production by 25% • Reduce lead-times and time-to-market for new products and technologies by 30%
Catalysis	• Accelerate the catalyst discovery process • Develop catalysts with selectivity approaching 100%

rely on various catalytic steps. Goals outlined in the *Catalysis Report* will help the industry realize significant process improvements. For example, if all catalytic processes associated with the top 50 chemicals were raised to their maximum process yields, total energy savings would exceed an estimated 0.47 quads per year.

Bioprocessing and biocatalysis will become increasingly important in the coming decades as lower energy and more environmentally friendly process methods are developed. The biocatalysis roadmap outlines the R&D needed to increase the use of bioprocessing in the chemical industry.

The development of new **materials,** such as synthetic polymers and composites, has fueled the growth of the chemical industry. These materials are used to create products with lower weight, better energy efficiency, higher performance and durability, and increased flexibility. Two new roadmaps, *Materials Technology* and *Materials of Construction,* outline goals for the further enhancement of new materials technology and materials used in the construction of processing equipment.

Separations, reaction engineering, and chemical measurements are critical elements of **process science and engineering.** Separation processes underlie virtually all aspects of the production process. Additionally, separation processes account for nearly two-thirds of the industry's process energy consumption. *Vision 2020:* 2000 Separations Roadmap identifies R&D needs in eight separation technologies: adsorbents, crystallization, distillation, extraction, membranes, separative reactors, bioseparations, and dilute solutions. Reaction engineering covers reactor design and scale-up, chemical mechanisms, and new reactor development. Addressing these research needs should result in optimized, integrated reactor systems with higher selectivity, yield, and purity. **Chemical measurements** are needed to characterize, monitor, and control chemical processes. Although no roadmap has been developed, a workshop has been held to define future R&D needs in this area.

Computational technologies are used in many aspects of chemical R&D, design, and manufacturing and have a broad range of applications—from molecular modeling to process simulation and control. The industry has developed roadmaps in two computational technology areas: computational chemistry and computational fluid dynamics. The impact of advances in these areas could be dramatic: reduced plant downtime, quicker progression from R&D to market, increased efficiency, and more reliable designs.

...AND IDENTIFY RESEARCH TO ACHIEVE THOSE TARGETS.

PERFORMANCE TARGET AREA COMPUTATIONAL FLUID DYNAMICS	0-5 Years	5-10 Years
Experimental Validation	• Develop multiphase flow test beds	• Develop new experimental methods applicable to large scale flows • Enhance capability for analysis of results • Perform experimental validation at small scale • Conduct small and large scale separate effects tests
Phenomenology and Constitutive Relations	• Characterize/model dense phases (e.g., laminar/turbulent flows) • Characterize/model interactions between phases • Develop reliable turbulence closures for multiphase flows • Characterize boundary conditions and interactions (e.g., inlets and wall and interior surface interactions)	• Incorporate population balance • Develop chemistry models for volume and surface phenomena
Numerical Methods	• Characterize/model dense phase • Develop more efficient, accurate algorithms and solvers	• Incorporate complex geometry • Develop adaptive computational grids • Improve parallelization techniques • Model changing positions of a free surface • Develop relevant data sets for code verification and scaling

Team & Partnership Activities

ACTIVE INDUSTRY LEADERSHIP

Guided by the goals defined in *Technology Vision 2020* and the technology priorities described in the roadmaps, OIT's Chemical Industry Team works in partnership with industry, trade groups, other government agencies, and the academic community. By aligning interests and leveraging capabilities and resources, these groups are creating the momentum needed to increase the energy efficiency and competitive position of the U.S. chemical industry.

The industry has established an executive steering group to assist OIT in determining how best to align its research activities with industry goals. The expertise and guidance of the industry leaders on the steering committee are helping the Chemical Industry Team ensure that the chemical R&D portfolio yields the greatest benefits for the industry while contributing to national goals for improved energy efficiency and environmental quality.

AN EXTENSIVE R&D PORTFOLIO

Through the roadmapping process, industry has identified critical chemical R&D areas. OIT is now working with industry to advance research in those areas by soliciting proposals for relevant R&D projects. Industry experts perform technical reviews of proposals received and, based on their recommendations, OIT's Chemical Industry Team makes the final selection of projects for cost-shared funding.

Currently, OIT's Chemical Team portfolio includes 28 projects. These projects represent a wide range of R&D activities that support *Technology Vision 2020* and the industry's roadmaps. Some aim to improve enabling technologies, such as computations, while others explore the possibilities in new chemical sciences, such as new materials and chemical synthesis.

COOPERATIVE ACTIVITIES

Since the chemical industry's outputs form the building blocks for products in a variety of other industries, the Chemical Team encourages joint efforts with OIT's other Industries of the Future teams to meet its vision goals. Similarly, many of OIT's enabling technologies programs—those that can potentially benefit a wide range of industries—offer opportunities for cosponsored activities with the chemical industry. Recently, the Chemical Team joined forces with OIT's Petroleum Team to collaborate on projects and activities of mutual benefit, including:

- a Practical Minimum Energy study to explore opportunities for improving energy efficiency
- joint efforts in multiphase computational fluid dynamics
- communications activities through the American Institute of Chemical Engineers

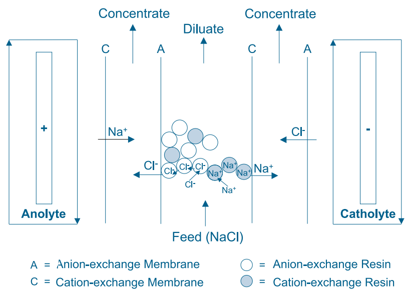
OIT's portfolio mix also includes activities, tools, and information to help the industry solve immediate competitive and environmental challenges. OIT's BestPractices programs provide support directly to companies with an emphasis on improving energy efficiency in the normal course of production.

REPRESENTATIVE CHEMICAL-RELATED PROJECTS IN OIT'S PORTFOLIO

	CHEMICAL SYNTHESIS	BIOTECHNOLOGY	MATERIALS	PROCESS SCIENCE & ENGINEERING	COMPUTATIONAL TECHNOLOGY
Chemical Team •Membrane for p-Xylene Separation			●	●	
•Direct Production of Silicones from Sand	●		●		
•Electrodeionization for Product Purification				●	
•Multi-Phase Computational Fluid Dynamics	●		●	●	●
•Sorbents for Gas Separations			●	●	
•Nanoscale Catalysts	●			●	
•Oxidative Cracking of Hydrocarbons to Ethylene	●		●	●	
•Selective Oxidation of Aromatic Compounds	●			●	
•Recovery of Thermoplastics via Froth Flotation			●	●	
•Catalytic Hydrogenation Retrofit Reactor	●			●	
•Separation of Hydrogen/Light Hydrocarbon Gases			●	●	
•Membrane Tube Module			●	●	
•Pressure Swing Absorbtion for Product Recovery				●	
•Alloys for Ethylene Reactors			●	●	
•Development of Non-Aqueous Enzymes	●	●			
•Chloro-Alkali Electrochemical Reactors	●			●	
•Plastics from Cellulose		●	●		
•Integrated Workbench for Gas-Phase Thermodynamics					●
•Instrumentation of Multiphase Flows					●
Combustion •NO_x Emissions Reduction by Oscillating Combustion				●	
•Radiation Stabilized Burner				●	
•Dilute Oxygen Combustion				●	
•Forced Internal Recirculation Burner				●	
Best Practices •Practical Minimum Energy	●	●	●	●	
•Plant-wide Assessments			●	●	
•Efficient Motor, Steam, Compressed Air, and CHP Systems				●	
Industrial Materials •Nickel Aluminides			●	●	
•Oxide Membranes			●	●	
•Metals Processing Laboratory			●	●	
Sensors & Controls •Intelligent Extruder			●	●	

See "Selected Chemical Portfolio Highlights" on the next two pages for additional information

Selected Chemical Portfolio Highlights



Electrodeionization combines ion exchange and electrodialysis to offer efficient, continuous operation.

AREA: PROCESS SCIENCE & ENGINEERING

PROJECT: **Electrodeionization for Product Purification**

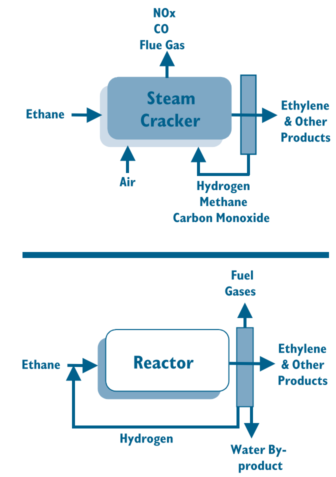
DESCRIPTION:

Electrodeionization, also called electrochemical ion exchange, has been recently established to make high-purity water for boiler feed, semi conductors, and pharmaceutical applications. To extend the use of this energy-efficient and non-polluting technology to the chemical industry, novel device technology is being developed and scaled up. Successful results will enable the direct deionization of chemical product streams economically, efficiently, and without creating waste salts:

- Potential energy savings of 5.3 x 1012 Btu in 2020
- Wasterwater reduction of 61.5 x 106 tons per year
- Avoides use of chemical regenerates

PARTNERS:

Argonne National Laboratory
EDSep, Inc.
The Purolite Company



The energy-efficient oxidative cracking process requires a reactor much smaller than a steam cracker.

AREA: CHEMICAL SYNTHESIS

PROJECT: **Oxidative Cracking of Hydrocarbons to Ethylene**

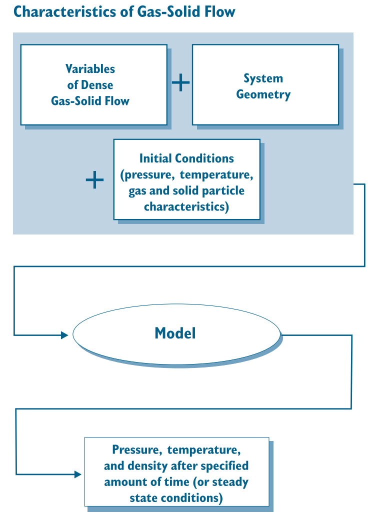
DESCRIPTION:

Production of ethylene by the traditional steam cracking process has been ranked as the single most energy-intensive process in the chemical industry. A new, internally fired process does not require a furnace, produces no flue gas, and eliminates decoking shutdowns. The simplified process produces the required olefin, along with water and small amounts of fuel gas.

- Eliminate NOx production
- Reduce carbon dioxide generation
- Save 11 to 15 trillion Btu annually by 2020
- Conserves resources

PARTNERS:

Sandia National Laboratory
Los Alamos National Laboratory
Dow Chemical Company
University of Minnesota
Reaction Engineering International



Computational models will predict characteristics of gas-solid flow to improve productivity in the petrochemical industry.

AREA: COMPUTATIONAL TECHNOLOGY

PROJECT: **Multiphase Computational Fluid Dynamics**

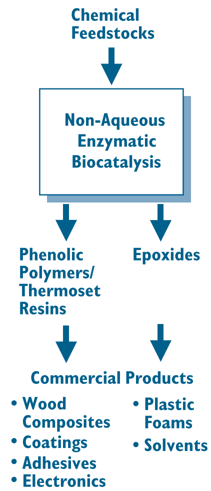
DESCRIPTION:

The Multiphase Fluid Dynamics Research Consortium was established to advance Computational Fluid Dynamics (CFD) beyond the state-of-the-art achievable by any single business or laboratory. The consortium's current projects include developing a computer model that can accurately predict dense gas-solid turbulent flow, which is the industry's highest priority for CFD modeling.

- Improves overall gas-solid flow operating capacity by as much as 90%
- Increases the capacity of existing gas-solid processes by 10-20%
- Increases industrial productivity

PARTNERS:

The consortium is a partnership among five DOE National Laboratories, seven universities, seven petrochemical companies, an energy equipment manufacturer, and a computer manufacturer.



Bioprocesses for polyphenols reduce waste generation and avoid the use of toxic solvents.

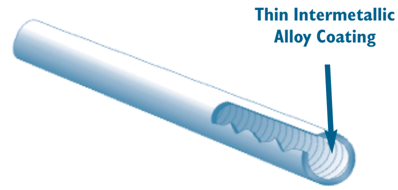
BIOTECHNOLOGY

Development of Non-Aqueous Enzymes

Chemical processes currently employed to produce phenolic polymers use formaldehyde, create undesirable by-products, or generate wastes that require treatment. Producing polyphenols through biocatalysis would enable manufacturers to significantly reduce costs and avoid disposal pre-treatments. Researchers are developing active and stable biocatalysts to carry out phenolic polymerization and to directly expodize propylene and other alkenes.

- Could save nearly 70 trillion Btu in 2020
- Higher yields with less waste
- Increased process efficiency

Massachusetts Institute of Technology
Oak Ridge National Laboratory
Rensselear Polytechnic Institute
University of California-Berkeley
Four chemical company collaborators



Alloy coatings are expected to reduce carburization and coke formation inside ethylene furnace tubes.

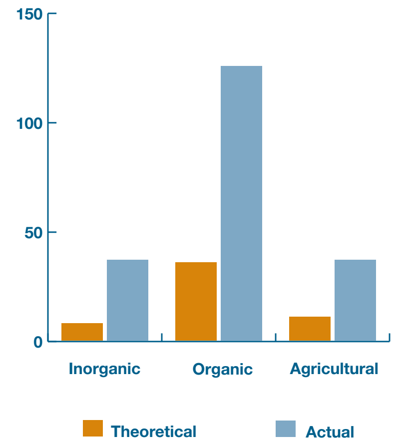
MATERIALS

Alloys for Ethylene Reactors

Coating the inside of ethylene furnace tubes with intermetallic alloy materials promises to reduce tube maintenance, a leading cause of inefficiency in ethylene production. Research is focusing on using these coatings to prevent two major problems with conventional tubes: carburization, which limits tube life, and coke formation, which requires costly plant shutdowns to steam decoke the tubes. Fabrication methods and welding techniques are also being developed.

- Longer tube service life
- Reduced furnace downtime
- Improved reaction conditions
- Lower energy use

Exxon Chemical Company
Shell Chemical Company
BP Amoco
Air Products and Chemicals, Inc.
Oak Ridge National Laboratory
Plus 6 other industry partners



Practical minimum energy use for selected chemical products and processes falls between the theoretical minimum and actual use.

BEST PRACTICES

Practical Minimum Energy Study

The objectives of this work are to develop baseline energy use for the manufacture of major chemicals and to determine the best and least energy-intensive way to manufacture those chemicals under practical operating conditions. The initial focus is on five chemical compounds within a single reaction class. Researchers will determine energy use in four different scenarios: theoretical; current practice; the most efficient combination of existing unit operations (processes); and the best practical combination of emerging unit operations. When completed for all top fifty chemicals, practical energy use minimums will assist decision-makers in developing energy management strategies and provide a useful comparison of energy needs across the chemical industry.

Bridges to Sustainability
University of Texas
University of Houston
North Carolina State University
Rice University

For more information on OIT's Chemical Portfolio, visit www.oit.doe.gov/chemicals